INTERPRETATION OF EPI SUITE™ MODEL RESULTS OF GLUCARIC ACID

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DATE:

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Interpretation of EPI Suite™ Model Results of Glucaric Acid

1.0 INTRODUCTION

US EPA EPI SuiteTM (version 4.11) is a publicly environmental fate and ecotoxicity screening-level predictive tool and does not take precedence over measured values. EPI SuiteTM consists of thirteen stand-alone environmental programs and one dermal adsorption program:

- AOPWIN estimates atmospheric oxidation rates
- BCFBAF estimates bioconcentration factor (BCF) and biotransformation rate (kM)
- BioHCwin estimates biodegradation of hydrocarbons
- BIOWIN estimates biodegradation probability
- ECOSAR estimates aquatic toxicity (LD₅₀, LC₅₀)
- HENRYWIN estimates Henry's law constant
- HYDROWIN estimates aqueous hydrolysis rates (acid-, base-catalyzed)
- KOAWIN estimates octanol-air partition coefficient
- KOCWIN estimates soil sorption coefficient (Koc)
- KOWWIN estimates octanol-water partition coefficient
- MPBPVP estimates melting point, boiling point, and vapor pressure (also referred to as MPBPWIN)
- WATERNT estimates water solubility (using atom-fragment methodology)
- WSKOW estimates water solubility (from log octanol-water partition coefficient)
- DERMWIN estimates dermal permeability coefficient (Kp), the dermally absorbed dose per event (DAevent) and Dermal Absorbed Dose (DAD) of organic compounds

The environmental fate, ecotoxicity and dermal absorption potential of glucaric acid (CASRN 87-73-0) were modelled and the outcomes are detailed below. The model outcomes are appended. The following information was used for the model predictions:

SMILES: OC(=O)C(O)C(O)C(O)C(O)C(=O)O

• CAS Num: 87-73-0



2.0 AOPWIN (Version 1.92)(Atmospheric Oxidation Program for Windows)

AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. It also estimates the rate constant for the gas-phase reaction between ozone and olefinic/acetylenic compounds. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals and ozone. AOPWIN is based upon the structure-activity relationship methods and incorporated updated fragment and reaction values.



3.0 BCFBAF (Version 3.01) (Bio-Concentration Factor / Bio-Accumulation Factor)

BCFBAF estimates the fish bioconcentration factor and its logarithm using two different methods. The first is the traditional regression based on log K_{OW} plus any applicable correction factors and is analogous to the WSKOW method. The second is the Arnot-Gobas method, which calculates BCF from mechanistic first principles. BCFBAF also incorporates prediction of apparent metabolism half-life in fish and estimates BCF and BAF for three trophic levels.



4.0 BioHCwin (Version 1.01) (Biodegradation Hydrocarbons program for Windows)

BioHCwin estimates the biodegradation half-life of petroleum hydrocarbons. This model uses a fragment-based approach.

5.0 BIOWIN (Version 4.10)

(Biodegradation program for Windows)

BIOWIN estimates the probability of rapid aerobic and anaerobic biodegradation of an organic compound in the presence of mixed populations of environmental microorganisms. The model contains seven separate models and the biodegradability estimates are based upon fragment constants.



6.0 ECOSAR (Version 1.11) (Ecotoxicity Structure Activity Relationships)

ECOSAR predicts the aquatic toxicity of chemicals based on their similarity of structure to chemicals with measured ecotoxicity values. The model considers correlates octanol/water partition coefficient (Kow) and aquatic toxicity. The model considers both neutral organic compounds and, if appropriate, specific chemical classes to further enhance the predictions.



7.0 HENRYWIN (Version 3.20) (Henry's Low Constant program for Windows)

HENRYWIN estimates the Henry's Law Constant (air-to-water partition coefficient) of organic compounds at 25°C. The Henry's Law Constant is predicted by two separate models which consider structural fragments: first, the Bond Contribution Method and second, the Group Contribution Method. HENRYWIN was unable to complete the Group Contribution Method as values were not available for all structural fragments.

8.0 HYDROWIN (Version 2.00) (Hydrolysis rate program for Windows)

HYDROWIN predicts the aqueous hydrolysis rate constants based on structural fragments for: esters, carbamates, epoxides, halomethanes, selected alkyl halides and phosphorus esters.

9.0 KOAWIN (Version 1.10) (K_{OA} octanol-air partition coefficient program for Windows)

KOAWIN predicts the octanol-air partition coefficient (K_{OA}) of an organic compound using the compound's K_{OW} and Henry's Law Constant. The K_{OA} is useful for predicting the partitioning behavior between air and environmental matrices such as soil, vegetation and aerosol particles.



10.0 KOCWIN (Version 2.00) (K_{OC} soil adsorption coefficient program for Windows)

KOCWIN predicts the ratio of the amount of chemical adsorbed per unit weight of organic carbon in the soil or sediment to the concentration of the chemical in solution. K_{OC} provides an indication of the extent to which a chemical partitions between solid and solution phases in soil. The K_{OC} predictions are based on either the Log K_{OW} value of the substance or based on Molecular Connectivity Index (MCI).



11.0 KOWWIN (Version 1.68) (K_{OW} octanol/water partition coefficient program for Windows)

KOWWIN predicts the logarithmic octanol-water partition coefficient of organic compounds. The model uses a "fragment constant" method in which a structure is divided into fragments and coefficient values of each fragment are summed together to yield the Log K_{OW} prediction.



12.0 MPBPVP (Version 1.43) (Melting Point, Boiling Point, Vapour Pressure)

MPBPVP predicts the boiling point (at 760 mmHg), melting point and vapour of organic compounds. The normal boiling point is predicted using a group contribution quantitative structure activity relationship. The melting point is estimated based on chemical structure and the boiling point of the substance. The vapour pressure is estimated based upon the normal boiling point of the substance.

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13.0 WATERNT (Version 1.01) (Water Solubility Program)

WATERNT predicts the water solubility of organic compounds at 25°C. The model estimates water solubility based on structural fragments.

14.0 WSKOW (Version 1.42) (Water Solubility K_{OW})

WSKOW predicts the water solubility of organic compounds based on the compounds Log Kow.

15.0 DERMWIN (Version 2.02) (Dermal program for Windows)

DERMWIN predicts the dermal permeability coefficient (Kp), the dermally absorbed dose per event (DAevent) and Dermal Absorbed Dose (DAD) of organic compounds via water contact. The model correlates Log K_{OW} and dermal permeability of a substance.

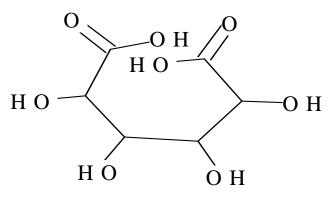


DISCLAIMER

is a global leader in delivering expert scientific, toxicological, engineering, and regulatory consulting services
that help companies to assess the safety and sustainability of their products, processes and assets, and to understand and comply with a variety of
regulatory approval and reporting requirements. provided this report solely for the purpose stated herein. The information contained in this
report was prepared and interpreted exclusively for the client and may not be <u>used in</u> any manner by any other party.
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of care whether based in negligence or otherwise, in relation to the use of this report in whole or in part by any third party. Any alternate use, including
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accepted practice and usual standards of thoroughness and competence for the professions of scientific assessment and regulatory affairs to assess
and evaluate information acquired during the preparation of this report. Any information or facts provided by others, and referred to or utilized in
the preparation of this report, is believed to be accurate without any independent verification or confirmation by This report is based upon
and limited by circumstances and conditions stated herein, and upon information available at the time of the preparation of the report.
undertakes not to use any non-plausible information or any information it has reason to believe is not accurate.

ATTACHMENT A

AOPWIN (VERSION 1.92) (ATMOSPHERIC OXIDATION PROGRAM FOR WINDOWS)

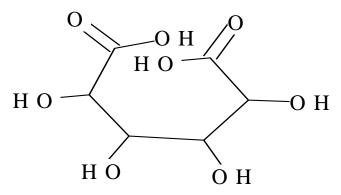


SMILES : OC(=0)C(0)C(0)C(0)C(0)C(=0)O CHEM : Glucaric acid MOL FOR: C6 H10 O8 MOL WT : 210.14



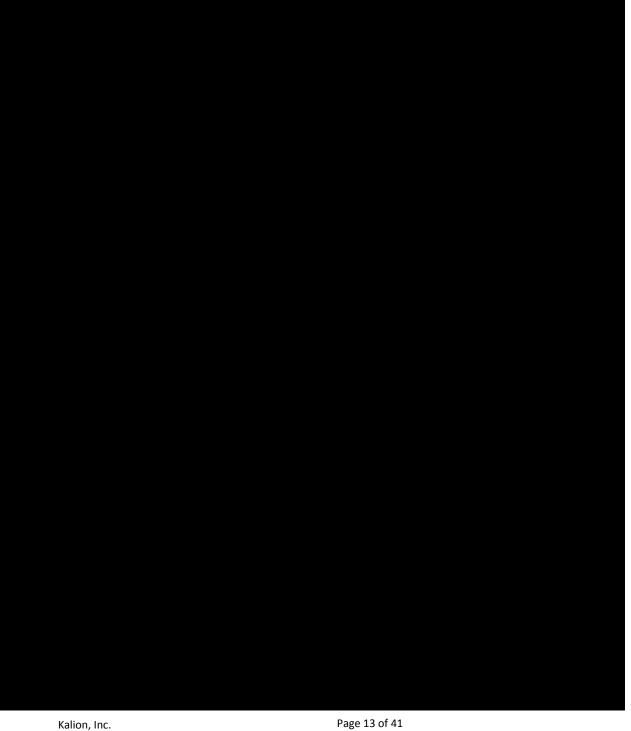
ATTACHMENT B

BCFBAF (VERSION 3.01) (BIO-CONCENTRATION FACTOR / BIO-ACCUMULATION FACTOR)



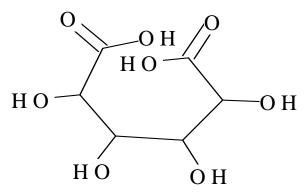
SMILES : OC(=0)C(0)C(0)C(0)C(0)C(=0)O
CHEM : Glucaric acid

CHEM : Glucaric ac MOL FOR: C6 H10 O8 MOL WT : 210.14



ATTACHMENT C

BIOHCWIN (VERSION 1.01) (BIODEGRADATION HYDROCARBONS PROGRAM FOR WINDOWS)



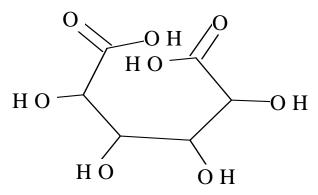
SMILES : OC(=0)C(0)C(0)C(0)C(0)C(=0)O
CHEM : Glucaric acid

CHEM : Glucaric acid MOL FOR: C6 H10 O8 MOL WT : 210.14

----- BioHCwin v1.01 Results -----

ATTACHMENT D

BIOWIN (VERSION 4.10) (BIODEGRADATION PROGRAM FOR WINDOWS)



SMILES : OC(=0)C(0)C(0)C(0)C(0)C(=0)O
CHEM : Glucaric acid

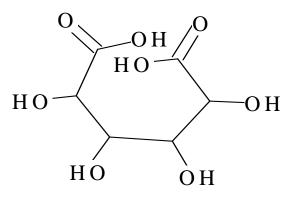
CHEM : Glucaric ac MOL FOR: C6 H10 O8 MOL WT : 210.14

----- BIOWIN v4.10 Results -----



ATTACHMENT E

ECOSAR (VERSION 1.11) (ECOTOXICITY STRUCTURE ACTIVITY RELATIONSHIPS)

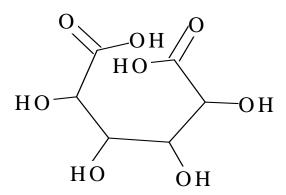


ECOSAR Version 1.11 Results Page



ATTACHMENT F

HENRYWIN (VERSION 3.20) (HENRY'S LOW CONSTANT PROGRAM FOR WINDOWS)



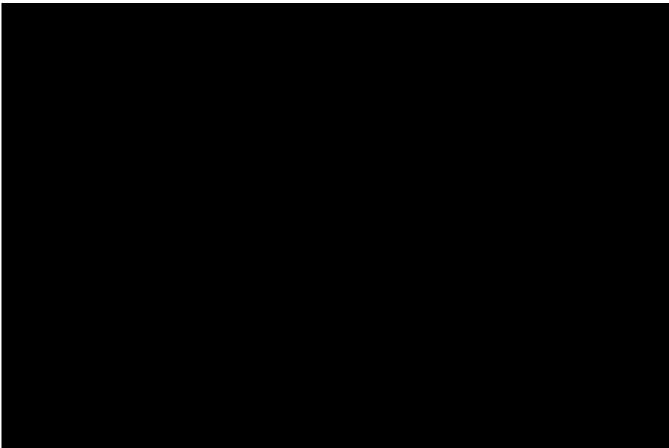
Bond Est : 3.10E-013 atm-m3/mole (3.14E-008 Pa-m3/mole)

Group Est: Incomplete

 $\texttt{SMILES} \ : \ \mathsf{OC}(=\mathsf{O})\,\mathsf{C}(\mathsf{O})\,\mathsf{C}(\mathsf{O})\,\mathsf{C}(\mathsf{O})\,\mathsf{C}(\mathsf{O})\,\mathsf{C}(\mathsf{O})\,\mathsf{C}(=\mathsf{O})\,\mathsf{O}$

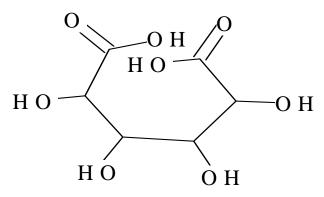
CHEM : Glucaric acid MOL FOR: C6 H10 O8 MOL WT : 210.14

----- HENRYWIN v3.20 Results -----



ATTACHMENT G

HYDROWIN (VERSION 2.00) (HYDROLYSIS RATE PROGRAM FOR WINDOWS)



SMILES : OC(=0)C(0)C(0)C(0)C(0)C(=0)O
CHEM : Glucaric acid

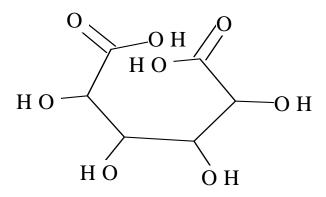
CHEM : Glucaric ac MOL FOR: C6 H10 O8 MOL WT : 210.14

----- HYDROWIN v2.00 Results -----



ATTACHMENT H

KOAWIN (VERSION 1.10) (KOA OCTANOL-AIR PARTITION COEFFICIENT PROGRAM FOR WINDOWS)



Log Koa: 8.39

SMILES : OC(=O)C(O)C(O)C(O)C(O)C(=O)O

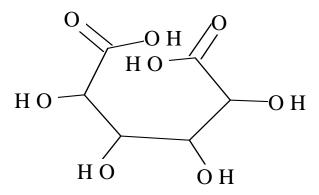
CHEM : Glucaric acid MOL FOR: C6 H10 O8 MOL WT : 210.14

----- KOAWIN v1.10 Results -----



ATTACHMENT I

KOCWIN (VERSION 2.00) (KOC SOIL ADSORPTION COEFFICIENT PROGRAM FOR WINDOWS)



SMILES : OC(=0)C(0)C(0)C(0)C(0)C(=0)O
CHEM : Glucaric acid

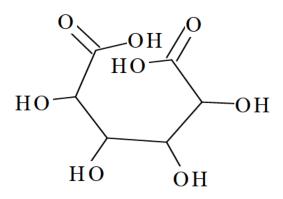
MOL FOR: C6 H10 O8

Koc may be sensitive to pH!
----- KOCWIN v2.00 Results -----

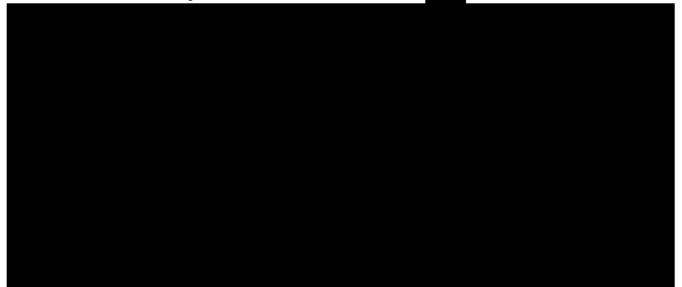


ATTACHMENT J

KOWWIN (VERSION 1.68) (KOW OCTANOL/WATER PARTITION COEFFICIENT PROGRAM FOR WINDOWS)

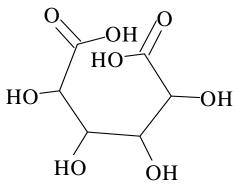


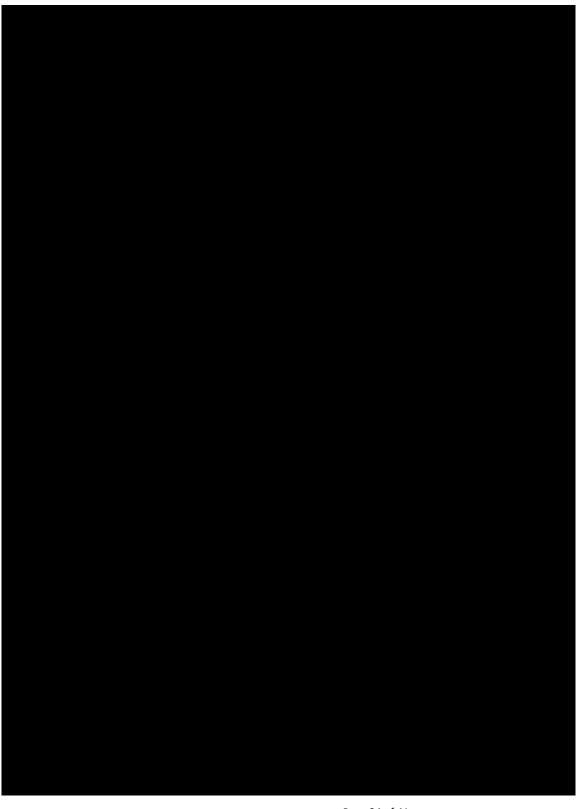
Log Kow(version 1.68 estimate):



ATTACHMENT K

MPBPVP (VERSION 1.43) (MELTING POINT, BOILING POINT, VAPOUR PRESSURE)

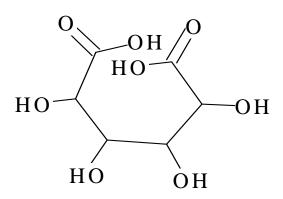






ATTACHMENT L

WATERNT (VERSION 1.01) (WATER SOLUBILITY PROGRAM)

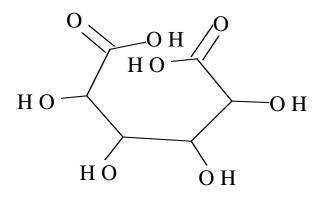


Water Sol (v1.01 est):



ATTACHMENT M

WSKOW (VERSION 1.42) (WATER SOLUBILITY KOW)

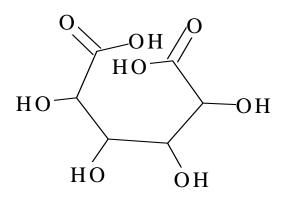


Water Sol:



ATTACHMENT N

DERMWIN (VERSION 2.02) (DERMAL PROGRAM FOR WINDOWS)



Kp (est):

CAS No.: 000087-73-0

SMILES : OC(=O)C(O)C(O)C(O)C(O)C(=O)O

CHEM : Glucaric acid MOL FOR: C6 H10 O8

